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PHASE TRANSFORMATIONS AND NONEQUILIBRIUM INTERFACES IN ALLOYS.(U)
SEP 79 J S LANGER, R F SEKERKA F44620-76-C-0103
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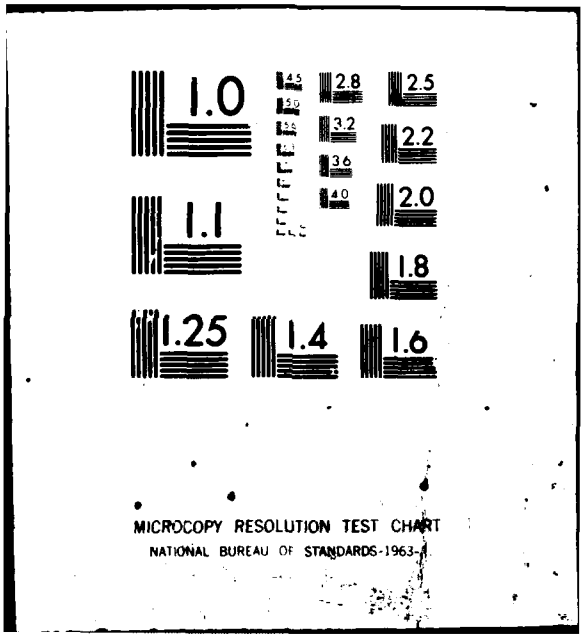
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Final Technical Report to AFOSR

Agreement number: F44620-76-C-0103

Principal Investigators: J. S. Langer and R. F. Sekerka
Carnegie-Mellon University, Pittsburgh, PA 15213

Title: Phase Transformations and Nonequilibrium Interfaces in Alloys

Grant Period: June 15, 1976 through September 30, 1979

I. Research Accomplishments

The following is a summary list of major research accomplishments during the period of this award. More detailed descriptions may be found in annual technical reports, renewal proposals, and in the publications listed in Section III.

A. Development of a new theory of dendritic solidification: Our new stability theory of dendritic crystal growth appears to be an important advance in the science of solidification. Major accomplishments include:

1) A quantitative theory of the dynamics of sidebranching deformations.
2) Development of a marginal-stability hypothesis which leads to a first-principles prediction of dendritic growth rates.
3) Application of this theory to the study of dendritic growth in dilute solutions.
4) Preparation of a review article on interfacial instabilities and crystal growth to appear in Reviews of Modern Physics.

Relevant publications are numbered 1-7, 9, 13 in Section II.

B. Studies in the theory of directional solidification: This project has focused primarily on the nonlinear theory of cellular solidification fronts. We have succeeded in demonstrating the existence of fully stable cellular structures in one model, and have also explored the behavior of this model in the extreme nonlinear regime. This work recently has led to new results in the theory of eutectic solidification.

Portions of this research are reported in Section V of publication no. 9. More detailed reports will be prepared shortly.

C. Numerical solutions of free-boundary problems: This work has been carried out in collaboration with Professor George Fix of the CMU Mathematics Department and has been supported primarily by CMU's Center for the Joining of Materials. However, the AFOSR contract made substantial contributions to this project during 1978-79. The goal of this project is the development of direct numerical methods for computing the motion of nonequilibrium liquid-solid interfaces under conditions when these interfaces may become morphologically unstable, as in dendritic growth. As a byproduct of this investigation, an AFOSR-supported student has developed and tested a computer program which models welding processes.

The major results of these calculations for the case of an unstable system are reported in publications numbered 11 and 12.

D. Kinetics of phase separation: Our program in precipitation kinetics has focused on both unstable "spinodal" systems and metastable nucleation problems. For solid alloy systems, we have developed a computational method based on the Langer-Baron-Miller (LBM) theory for predicting small-angle X-ray scattering intensities as measured during heat treatments involving experimentally realistic sequences of temperature variations. We also have incorporated hydrodynamic effects into the LBM theory in order to investigate phase separation in binary fluid mixtures. Most recently, we have developed a combined nucleation-growth theory which seems to account quite well for previously unexplained experimental results in near-critical fluid systems.

Relevant publications are nos. 8 and 10.

II. Publications

1. J. S. Langer and H. Müller-Krumbhaar, "Stability Effects in Dendritic Crystal Growth", J. Crystal Growth 42, 11 (1977).
2. J. S. Langer and H. Müller-Krumbhaar, "Theory of Dendritic Growth I: Elements of a Stability Analysis", Acta Metallurgica 26, 1681-1687 (1978).
3. J. S. Langer and H. Müller-Krumbhaar, "Theory of Dendritic Growth II: Instabilities in the Limit of Vanishing Surface Tension:, Acta Metallurgica 26, 1689-1695 (1978).
4. H. Müller-Krumbhaar and J. S. Langer, "Theory of Dendritic Growth III: Effects of Surface Tension", Acta Metallurgica 26, 1697-1708 (1978).
5. J. S. Langer, R. F. Sekerka, and T. Fujioka, "Evidence for a Universal Law of Dendritic Growth Rates", J. Crystal Growth 44, 414-418 (1978).
6. J. S. Langer, "Interfacial Instabilities and Dendritic Crystal Growth", Progress of Theoretical Physics, Supp. No. 64, 463 (1978).
7. J. S. Langer, "Dendritic Solidification of Dilute Solutions", to be published in Physicochemical Hydrodynamics.
8. A. Schwartz, "Hydrodynamic Effects on Spinodal Decomposition in a Binary Fluid", submitted to Physical Review A.
9. J. S. Langer, "Instabilities and Pattern Formation in Crystal Growth", to be published in Reviews of Modern Physics, January 1980.
10. J. S. Langer and A. Schwartz, "Kinetics of Nucleation in Near-Critical Fluids", to be published in Physical Review A.
11. Jeffrey B. Smith and J. S. Langer, "Numerical Methods in Solidification Theory", Proceedings of the Third Moscow Conference on Collective Phenomena, to be published by the New York Academy of Sciences.
12. Jeffrey B. Smith, "Shape Instabilities and Pattern Formation in Solidification: A New Method for Numerical Solution of the Moving Boundary Problem", submitted to the Journal of Computational Physics.
13. H. Müller-Krumbhaar and J. S. Langer, "Sidebranching Instabilities in a Two-Dimensional Model of Dendritic Solidification", in preparation.

III. Interactions

The following is a list of invited talks, presented at scientific conferences or at other laboratories, in which research performed under this contract was described.

Lectures presented by J. S. Langer on kinetics of phase separation:

University of Toronto, Physics Colloquium, March 10, 1977.
Symposium on Order and Disorder in Solids, Paris, July 1977.
Materials Science Colloquium, University of California, Los Angeles, January 1978.
Research Institute for Fundamental Physics, Kyoto, July 17, 1978.
University of Hannover, W. Germany, May 21, 1979.
Université Libre, Brussels, May 23, 1979.
Köln University, W. Germany, May 25, 1979.
Aspen Center for Physics, August 1979.
Mid-West Solid-State Physics Conference, Columbus, Ohio, Oct. 9, 1979.
Oak Ridge National Laboratory, November 7, 1979.

Lectures presented by J. S. Langer on solidification theory:

Gordon Conference, July 19-23, 1976
University of Toronto Metallurgy Colloquium, March 8, 1977.
Moscow Seminar on Collective Phenomena, April 18, 1977.
Harvard University, Theoretical Physics Seminar, May 12, 1977.
IBM Research Laboratory, May 17, 1977.
International Conference on Crystal Growth 5, Boston, July 19, 1977.
Cornell University, November 17, 1977.
Stanford University, January 5, 1978.
Midwinter Solid-State Research Conference, Laguna Beach, California January 12, 1978.
University of California, Irvine, January 13, 1978.
Ames Laboratory, Iowa State University, March 31, 1978.
Chicago Area Solid-State Colloquium April 12, 1978.
International Symposium on Nonlinear Nonequilibrium Statistical Mechanics, Kyoto, Japan, July 13, 1978.

Lectures presented by J. S. Langer on solidification theory (continued):

Physiocochemical Hydrodynamics Conference, Washington, D.C., November 7, 1978.

National Bureau of Standards, Washington, D.C., November 16, 1978.

City College, New York, December 13, 1978.

Statistical Mechanics Conference, Rutgers University, December 14, 1978.

International Conference on Collective Phenomena, Moscow, USSR, December 27, 1978

Symposium of the Division of Condensed Matter Physics, American Physical Society, Chicago, March 21, 1979.

Bell Telephone Laboratories, May 1, 1979.

Greater Washington Area Solid-State Physics Colloquium, October 4, 1979.

Lectures presented by R. F. Sekerka on solidification theory and nonequilibrium interfaces:

Darken Conference, U.S. Steel Corporation, Monroeville Pa., August 1976.

University of Illinois, Urbana, March 1977.

National Bureau of Standards, Washington D.C., May 1977.

IBM Laboratories, Yorktown Heights, June 1977.

Michigan Technological University, Houghton, May 1978.

American Assoc. of Crystal Growth, Gaithersburg Md., July 1978.

Third European Symposium on Materials Science in Space, Grenoble, April 1979.

AIME Meeting, Milwaukee, September 1979.

IV. Personnel

Principal Investigator: J. S. Langer

Co-Principal Investigator: R. F. Sekerka

Postdoctoral Research Associates:

- H. Müller-Krumbhaar (1976-77)
- A Schwartz (1978-79)
- J. Smith (partial support, 1978-79)

Research Assistants:

- K. Kasturi (Thesis student, quit for personal reasons, 1976-78.)
- P. Popper (Pre-qualifying student 1977.)
- R. Mathur (Thesis student, should complete Ph.D in 1980-81.)
- V. Datye (Thesis student, should complete Ph.D in 1981.)

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Dendritic crystal growth, cellular solidification fronts, precipitation kinetics, interfacial instabilities, nucleation, free-boundary problems

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

This report describes progress in research on phase transformations and nonequilibrium interfaces achieved during the period June 15, 1976 to September 30, 1979. Major accomplishments include the development of a theory of dendritic crystal growth and performance of calculations pertaining to phase separation in alloys and fluid mixtures.

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